

Docusate sodium

577-11-7 | DTXSID8022959

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.19\text{e-}11$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.22\text{e-}01$

**Confidence level:**  $8.32\text{e-}01$

## Nearest Neighbors from the Training Set

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Isoproturon

**Measured:**  $1.20\text{e-}11$

**Predicted:**  $3.23\text{e-}11$

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Bornyl acetate

**Measured:**  $1.39\text{e-}11$

**Predicted:**  $1.36\text{e-}11$

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

**Measured:**  $4.80\text{e-}11$

**Predicted:**  $4.73\text{e-}11$

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Dimethyl adipate

**Measured:**  $8.40\text{e-}12$

**Predicted:**  $6.84\text{e-}12$

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Dimethyl glutarate

**Measured:**  $3.30\text{e-}12$

**Predicted:**  $3.76\text{e-}12$